Direct Observation of the α-ε Transition in Shock-Compressed Iron via Nanosecond X-ray Diffraction

Kai Kadau, T-14; Timothy C. Germann, X-1; Peter S. Lomdahl, T-14; Brad L. Holian, X-1; D.H. Kalantar and J. Hawreliak, Lawrence Livermore National Laboratory; K. Rosolankova and J.S. Wark, University of Oxford

One of the most fundamental properties of a solid is its crystallographic structure. Many crystals undergo structural phase transitions under the influence of static pressure or shock compression. One of the most studied systems at high pressure is iron because of its technological importance in society and its geophysical role within the earth's core.

This joint effort of small-scale experiments and large-scale atomistic simulations shows the first direct measurement of a structural transformation in shocked iron, in situ, and with nanosecond resolution [1]. These results are in remarkable agreement with the theoretical predictions on the transformation mechanisms of the α → ε [body-centered cubic (bcc) → hexagonal close-packed (hcp)] phase transformation in solid iron single crystals given by K. Kadau, et al. [2]. This work provides an excellent example of how theoretical methods can guide experiments and shows the convergence of large-scale theoretical techniques such as atomistic simulations and small-scale experiments on the other side. Further experiments to compare shocks to atomistic predictions [3] for shocks along [011] and [111] are underway.

For more information contact Kai Kadau at kkadau@lanl.gov.

[1] D.H. Kalantar, et al., *Phys. Rev. Lett.* **95**, 075502 (2005).
[2] K. Kadau, et al., *Science* **296**, 1681 (2002).
[3] K. Kadau, et al., *Physical Review B* **72**, 064120 (2005).

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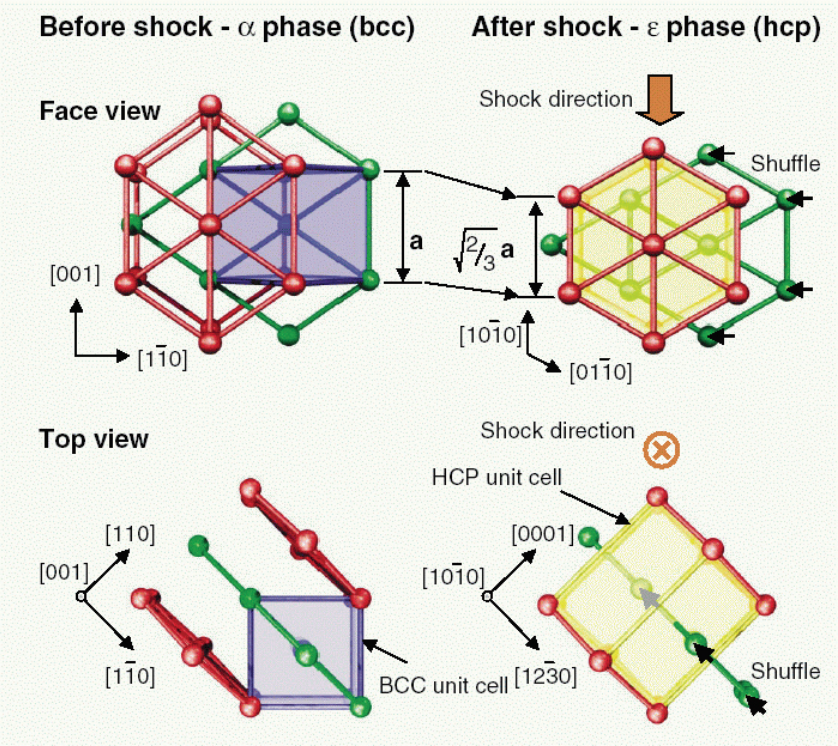

Fig. 1.
Schematic showing the lattice structure of the bcc and hcp phase for iron. A pseudohexagonal structure results from the 18.4% compression of a bcc lattice along [001]. Shuffling of alternate (110) planes creates the close-packed structure.

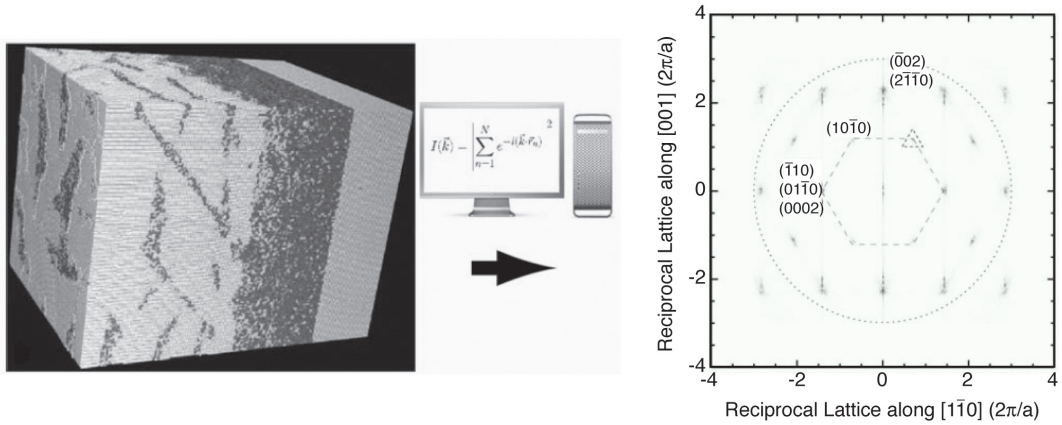

Fig. 2.
This figure shows schematically the method of post processing the molecular dynamics data in order to compare to experimental diffraction data. The atomic positions from the atomistic simulation are Fourier transformed into reciprocal lattice space, so the high intensity peaks represent diffraction planes in the crystal structure. The units are based on the inverse of the original cubic bcc cell. Three points are labeled with the plane labels on the figure. One point contains three labels, to show that there is a bcc component and two hcp components, due to the two degenerate hcp states. A dashed hexagon shows the reciprocal lattice points are approaching a hexagon. The dotted circle gives the limits that can be probed using K-shell radiation from an iron backlighter.

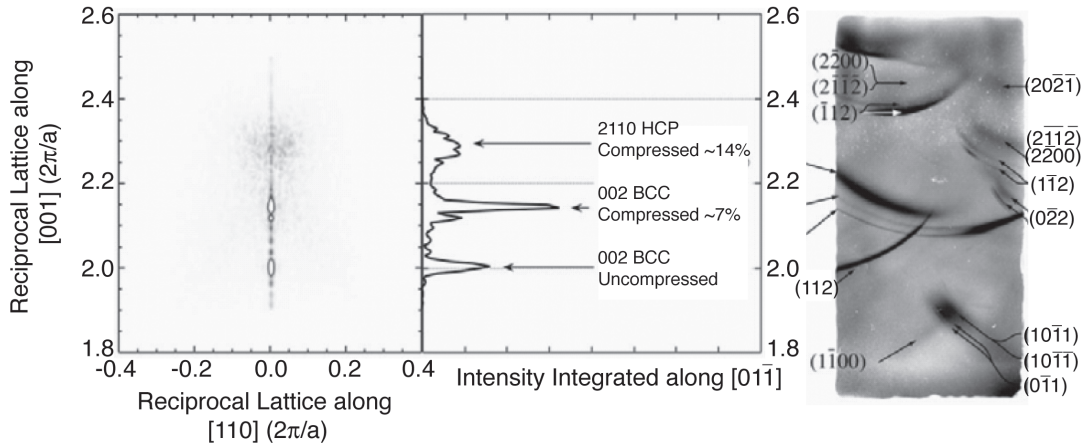

Fig. 3.
A high-resolution image of the bcc (002) and hcp (2-1-10) peaks. It also shows the integration over the [1-10] direction to give an idea of the widths of the representative peaks. Arrows show the location on experimental film the measurement of each of these peaks. Other diffraction planes are labeled with their plane labels, in both bcc and hcp.